Chapter 7
What Does It Mean for a Singularity to be Resolved?

We have now seen and studied in quite some detail a general mechanism by which loop quantum cosmology can resolve singularities, based on the fundamental difference equation, and a very specific one of an effective bounce in a solvable model. In such a situation, and also in comparison with Wheeler–DeWitt quantizations, the question arises what it should mean, in general, for a singularity to be resolved.

The general issue is rather messy due to the presence of several different statements even in the classical determination of singularities. One may use curvature divergence as a physical condition known from many explicit solutions, but one difficult to handle at a general level. Strict theorems mainly make use of the comparatively weak and rather different notion of geodesic incompleteness. When potential resolutions of singularities are to be discussed, the first question to ask is which one of the classical criteria for a singularity one should focus on.

Another important condition to be considered is the genericness of resolution mechanisms. Singularities can be avoided even classically by clever choices of initial values [1]. The classical singularity problem does not state that all realistic solutions must develop singularities; the problem is rather caused by the fact that no mechanism is known that could avoid singularities generically. Genericness is also the most important condition for quantum cosmological resolutions of singularities; also here it is not that difficult to avoid specific types of singularities since the freedom, for instance in violating energy conditions, is much higher than classically.

7.1 Density Bounds

We have already encountered bounds for the quantum density ρ_Q in the context of the quantum Friedmann equation; see the remarks after (6.32). Since there are quantum corrections from fluctuations and higher moments in the expression (6.33) for the quantum density, the physical matter density that follows from the quantum matter Hamiltonian may still be unbounded in non-semiclassical states. For stronger results about density bounds, the matter density must be constrained by additional means, probably involving the dynamics of specific models.

DOI: 10.1007/978-1-4419-8276-6_7,

An alternative result exists for models with a cosmological constant in addition to the free, massless scalar. These models are not harmonic, but have one advantage compared to general matter systems because they are still deparameterizable by φ. If one considers the spectrum of a density operator defined by quantizing the matter energy divided by the volume with inverse-volume techniques of loop quantum gravity, on upper bound for density values can be obtained [2].

Although a rigorous derivation is important, the existence of such a bound is not altogether surprising [3, 4]. The loop modification of c by $\sin(\delta c)/\delta$ replaces the unbounded c by a bounded function. Unless quantum back-reaction is strong, the matter density is then bounded by the Friedmann equation. The non-trivial aspect of loop quantum cosmology is not to bound the density in isotropic models, but to construct consistent embeddings of such models in a full quantum system that includes inhomogeneities. Such an embedding has not yet been achieved completely consistently, but the relationship between loop quantum cosmology and loop quantum gravity is showing the available possibilities.

Upper bounds for the spectrum of density operators can be interpreted as one contribution to the resolution of singularities. However, they also show the limitations of some of the current results obtained in loop quantum cosmology. In isotropic models one can easily construct density operators, once methods for inverse-triad quantizations are known following [5]. But in inhomogeneous situations or the full theory there is no well-defined way to obtain density operators in loop quantum gravity; only quantities of density weight zero can be quantized. One may thus quantize the matter Hamiltonian $\hat{H}$ [6] and the volume $\hat{V}$ [7, 8] corresponding to some finite region. Their expectation values in a given state then provide a measure for the density $\langle\hat{H}\rangle/\langle\hat{V}\rangle$. One can use the same construction in isotropic models, which would bring the results closer to those of the full theory. An alternative expression for the matter density results, one that differs from the expectation value $\langle\widehat{HV^{-1}}\rangle$ of an isotropic density operator. The difference is given by moments of the state, and is strong in a highly quantum state. If the moments of the state are large, the physical matter density may be unbounded even if there is an upper bound on the spectrum of density operators. To decide whether actual densities are bounded, one must bring the moments and the shape of states under better control. No general, state-independent bounds as in [2] can be expected. Not many results in this direction are known, but it has already been demonstrated numerically that the bounds of [2] can be breached if the shape of states is taken into account [9].

7.2 Bounces

A more specific scenario for singularity resolution is a turn-around of a from collapse to expansion, or a bounce [10], keeping the scale factor away from zero and energy densities finite.

Example 7.1. (*Fluctuation-triggered bounce*) In a Wheeler–DeWitt treatment of the model analyzed in Example 2.1, the requirement of self-adjointness in the face of a boundary of the a-axis requires special fall-off conditions for wave functions. The wave function is always suported on $a > 0$, which implies that the expectation value of $\hat{a}$ cannot become zero. In contrast to the classical solutions, a bounce or at least a mechanism to keep $\langle\hat{a}\rangle$ away from the singular $a = 0$ is indicated.

In order to see the role of the boundary more clearly, we use effective equations for the system quantized with the non-canonical variables V and $D = VP$, $\{V, D\} = V$. As discussed in Sect. 2.2, group-theoretical quantization then leads to self-adjoint basic operators on the phase space $\mathbb{R}^+ \times \mathbb{R}$. In Example 2.1 we reformulated the system in Schrödinger form in the presence of dust, for which the Hamiltonian, when quantized by our non-canonical operators, can be taken to be of the self-adjoint form $\hat{H} = \hat{V}^{-1}\hat{D}^2\hat{V}^{-1}$. (By contrast, $\hat{H} = \hat{P}^2$ is not self-adjoint on the positive half-plane.) In the affine variables, the Hamiltonian is no longer quadratic and requires a choice of factor ordering, here done in a simple (but non-unique) symmetric way. The dynamics is no longer of free-particle form, resolving the problem of wave packets crossing the boundary seen in Example 2.1.

In order to determine the role of fluctuations at small volume, we perform a background-state expansion and then compute an expectation value of the Hamiltonian, or use the methods of Chap. 13. To second order, we obtain the quantum Hamiltonian

$$H_Q = \frac{\langle\hat{D}\rangle^2}{\langle\hat{V}\rangle^2} + \frac{1}{\langle\hat{V}\rangle^2}(\Delta D)^2 - 4\frac{\langle\hat{D}\rangle}{\langle\hat{V}\rangle^3}\Delta(VD) + 3\frac{\langle\hat{D}\rangle^2}{\langle\hat{V}\rangle^4}(\Delta V)^2. \qquad (7.1)$$

Fluctuation terms clearly change the Hamiltonian and, when large, can affect the dynamics. For instance, for a state that remains unsqueezed Gaussian at small scales we have $\Delta(VD) = 0$ and $(\Delta D)^2 = \langle\hat{V}\rangle^2\hbar^2/4(\Delta V)^2$. (The uncertainty relation, saturated for a Gaussian, follows as in the discussion of harmonic cosmology; see Chap. 13 for details.) For such states, we can write

$$H_Q = P^2\left(1 + 3\frac{(\Delta V)^2}{\langle\hat{V}\rangle^2}\right) + \frac{1}{4}\frac{\hbar^2}{(\Delta V)^2} = p_T \qquad (7.2)$$

with the dust momentum p_T equal to the Hamiltonian in this deparameterization. We have transformed back to the conventional curvature parameter P, now defined as $\langle\hat{D}\rangle/\langle\hat{V}\rangle$. Since there is no explicit T-dependence, p_T is conserved. Classically, it equals P^2 and is positive; thus, P or the time derivative of the scale factor cannot vanish and there is no bounce. With the fluctuation terms, there is a chance for P to vanish at non-zero p_T, in some cases corresponding to an extremum of a, provided fluctuations are significant. Fluctuations are dynamical, satisfying the equation $\mathrm{d}(\Delta V)^2/\mathrm{d}T = 4\langle\hat{D}\rangle(\Delta(VD)_2(\Delta V)^2/\langle\hat{V}\rangle)$, and the general behavior requires an analysis of the whole system coupling expectation values to fluctuations and correlations. In some examples, wave-function dynamics (for instance in the Bohmian viewpoint) has shown that bounces do arise [11–13].

Effective equations in some loop quantized systems show bounces that are not solely based on quantum fluctuations, but more importantly on quantum-geometry modifications. Such equations have not been derived yet in many models because the interacting nature of any common matter system in the presence of gravity makes this rather involved. But a solvable model has been identified, and it can be used as the basis for perturbation expansions. In such situations, which may be rather special but can be analyzed concretely, evidence for bounces has been seen. Assuming that a state remains sufficiently semiclassical at high densities and that matter is dominated by kinetic energy terms, the conclusion for a bounce to happen is rather robust. This conclusion can clearly be inferred from the perturbation equations we looked at before, which can also be extended to anisotropic or inhomogeneous situations. Sometimes one appeals to asymptotic properties, indicating that kinetic terms do become asymptotically dominant near a singularity since, in contrast to the potential in the energy density, they carry an inverse power of the scale factor. Also the Belinsky–Khalatnikov–Lifshitz (BKL) conjecture [14] may be taken to indicate that homogeneous models describe the approach to a singularity generically, in which case the dynamics for long stretches of time would be determined by the simple Bianchi I model. If the free massless scalar Bianchi I model would in general have bounces, one could expect this result to apply also to more generic situations.

But the very asymptotic regime used in this line of arguments is avoided by a bounce, which would imply that the universe never gets arbitrarily close to a singularity where kinetic domination or BKL-type arguments can be used. Theorems about asymptotic properties do not provide estimates of when exactly such a regime is reached, which could then be tested at the bounce. Even if this were possible, the presence of a bounce would become dependent on initial conditions since changing them would put the asymptotic regimes at different places. For these reasons, a kinetic-driven inhomogeneous bounce relying on asymptotic arguments such as the BKL conjecture cannot be generic.

Moreover, in these considerations one would still assume the quantum gravitational state to be sufficiently semiclassical. However, quantum back-reaction is in general important and can significantly change the behavior. Then, the classical theorems about the asymptotic dynamics would be uprooted and could no longer be used—the quantum system is one of many independent dynamical variables in coupled motion which must be re-analyzed for its asymptotic properties. Even if the time derivative of the scale factor approaches zero due to the action of some quantum repulsive force mediated by discrete geometry, quantum variables may not allow it to be precisely zero. In the effective Friedmann equation (6.34), for instance, we are comparing a density term, which in the solvable model vanishes at the bounce, with a correlation term. Even if one might have reason to expect quantum correlations to be small, if they are not exactly zero they would still be significant compared to zero.

In the big-bang phase, not just expectation values but also fluctuations, correlations and higher moments of a state are important. Effective equations describe this as a higher-dimensional dynamical system where quantum variables couple to expectation values. Such systems can have properties quite different from what a low-dimensional truncation might indicate. For instance, instead of bouncing sharply the scale factor could approach small sizes and linger there with nearly vanishing $\dot{a}$. But quantum fluctuations fluctuate, and so $\dot{a}$ may never be exactly zero as required for a

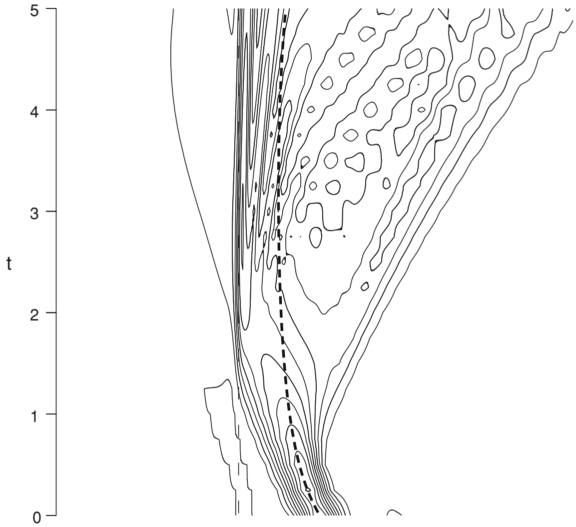

Fig. 7.1 A wave packet as a function of volume (horizontal) and time, bouncing, spreading and tunneling as indicated by the contours growing to the *right* (bouncing) and *left* (tunneling) [47]. (*Dashed*: expectation value, *long-dashed curve*: zero volume)

bounce; or it might become zero many times, resulting in repeated oscillations of a small universe. In principle it is even possible for a to approach the singular value zero asymptotically, despite the bound on energy density during kinetic domination. Different asymptotic behaviors resulting from the state dependence of evolution have been demonstrated in the Wheeler–DeWitt context [15, 16]. All these possibilities remain, at present, wide open. A general conclusion is much more difficult to reach than in the simple solvable model or in situations close to it.

Even if one could show the presence of a bounce generally, or at least in a sufficiently large class of models and situations, it would provide only a classical picture by an effective geometry. (In Chap. 10 we will discuss obstructions to the existence of effective line elements due to quantum-geometry effects in the presence of inhomogeneities.) Quantum effects would be included, for instance by holonomy corrections of geometry and by quantum back-reaction, but the effective bounce would only refer to the expectation value of a wave function. Repulsive forces of quantum geometry then erect a potential barrier which classical dynamics cannot penetrate. But quantum physics is rarely impressed by a barrier as long as it is of finite height. Wave functions can simply tunnel through (see Fig. 7.1), and if they reach $a = 0$ in this way one would again have to grapple with the singularity issue. Thus, the wave function must still be ensured to be non-singular in a fundamental rather than effective sense, based on the difference equation it has to obey.

At this point, we have to come back to the factor ordering in the Hamiltonian constraint, which was restricted by singularity removal based on the difference equation, but which was independently chosen in a particular form to make the free scalar model solvable. These orderings do not agree: using the solvable ordering for a fundamental singularity analysis would not allow one to evolve through $\mu = 0$, as can be seen by looking at the recurrence that follows from (5.20). The solvable ordering must be seen as an approximation, just as we had to ignore inverse-triad corrections to realize solvability. Re-ordering terms will introduce additional corrections which spoil the linear nature of the model, but which like ordinary interactions can be included perturbatively as long as quantum effects are not very strong.

Ultimately referring to the difference equation to study the singularity issue and to shed light on what came before the big bang makes us face the interpretational question of what time is in a deep quantum regime. It is unlikely to be a classically supported internal time such as φ or a, especially if deparameterizability is required to realize such a time choice. To cross quantum regimes, one might even have to switch to genuine quantum variables as time parameters which would have no classical analog [17, 18]. Covariances would indeed be a good choice since they are often monotonic when a state gets ever more squeezed. (Squeezing has in fact been related to entropy in several cosmological settings [19–25].) What the difference equation, essentially using as internal time the triad component (the scale factor squared with a sign for orientation), gives us as a picture for the transition through the classical singularity is a branch of a negatively oriented universe flipping to a positively oriented one, turning its inside out. This view is of particular interest if parity-violating matter is coupled to gravity, as this would strongly influence the transition and make the pre- and post-big bang phases differ in fundamental properties.

What the effective scenarios studied so far indicate, on the other hand, would be a bouncing trajectory with respect to some matter clock, which stays at one orientation of space but provides a minimum for volume. But this is borne out clearly only if one avoids strong quantum regimes by choosing a large matter content and large p_φ, making the universe kinetic-dominated at large volume where it can bounce easily by loop effects. In a deep quantum regime, single trajectories no longer matter; many different branches typically arise in superposition. Such a superposition can include both orientations of space, even for "times" which would all be considered as being before the big bang. Maybe there is not even a single notion of time that can explain the whole transition; time like geometry would have to emerge from the wave function. No such scenario for the emergence of time is available yet, but taken together all indications for the singularity removal in loop quantum cosmology show that this is what must be realized. Approaching the strong quantum regime with more refined techniques than are available now will open up access to this deep conceptual problem.

7.3 Quantum Cosmology

In the general setting of quantum cosmology, not using specific loop-quantization or other effects, singularity removal has been suggested and discussed in many different ways. None of these effects is as strong as the repulsive force arising from holonomy corrections in loop quantum cosmology, but subtle mechanisms sometimes exist. Due to the relative weakness, a conclusion about singularity removal here depends more strongly on interpretational issues of the wave function. See for instance [26] for a definition and analysis in the context of the consistent-histories formulation.

7.3.1 Interpretational Issues

Quantum cosmology plays a special role in quantum physics because the observer is always within the quantum system. The Copenhagen interpretation becomes inapplicable, but other options are available. Several of them have been claimed to be the only viable one in this context, most emphatically for the Bohmian viewpoint and the consistent-histories approach [27–29] (or even the many-worlds interpretation). The question of how to interpret quantum states is relevant for the singularity problem in quantum cosmology whenever arguments are based on typical quantum properties of wave functions rather than quantum-geometry effects. From this perspective, one can describe the main progress made by loop quantum cosmology as avoiding interpretational issues either by using quantum hyperbolicity for general wave functions, or by providing strong quantum-geometry effects.

In many applications of loop quantum cosmology, and in most parts of this book, one can take a pragmatic view. For observational aspects it is mainly the dynamics of expectation values and fluctuations that matters. Fluctuations, via quantum back-reaction, are then important for the dynamics, but not for the measurement problem where interpretational issues would strike with full force. It may even be possible to base the quantum-to-classical transition from fluctuations to matter perturbations in the early universe on quantum back-reaction of modes [30], but this problem still needs to be explained, perhaps by decoherence. (see also Sect. 10.4.1.)

7.3.2 Examples

If singularity resolution is to be based on aspects of wave functions, specific mechanisms require further input in addition to just a quantization scheme, as it has been done in the traditional proposals for initial conditions of a wave function by Vilenkin [31] and Hartle–Hawking [32]. This approach accepts the presence of a classically counterintuitive regime around the singularity, and replaces it with quantum notions such as tunneling or signature change, or outright quantum potentials [33]. Such schemes have primarily been formulated in isotropic models, and one often encounters difficulties when one tries to extend them to more general situations [34, 35]. Also future singularities have been discussed in this spirit [36]. In loop quantum cosmology, restrictions for states arise via dynamical initial conditions [37, 38].

Sometimes it is argued that quantization of a cosmological model with the positive scale factor a as the configuration variable resolves the singularity in the sense that a-expectation values of regular wave functions cannot be zero: any normalizable state must be supported at non-vanishing values of a, providing contributions to the expectation value which cannot completely cancel since no negative a are allowed. A minimum for a in the sense of expectation values may thus arise at small volume and strong curvature (where one may not trust Wheeler–DeWitt quantizations but rather prefer a loop quantization which then removes zero as the minimum for the basic geometrical variable p). The problem with this statement is that it depends on interpretational issues of the wave function as well as on implicit assumptions on the physical inner product. No explicit geometrical picture of how the singularity is resolved arises in this way, but it has been realized in some cases; see e.g. [39].

More specifically referring to quantum dynamics, quantum back-reaction provides additional terms to an effective Friedmann equation which should be imortant near $a = 0$. Some cases where a bounce at small volume ensues are indeed known [11–13, 15], not derived by the methods used in the preceding chapters but by explicit wave functions or a Bohmian formulation of quantum cosmology; see also the example at the beginning of this chapter. In this way, geometrical pictures of singularity resolution result which qualitatively can be compared with those of loop quantum cosmology. But the robustness in this case is much less investigated. In fact, at least the solvable Wheeler–DeWitt model analyzed before, which is free of quantum back-reaction, does not have a bounce. Whether or not singularities are removed by such a mechanism alone would thus depend on the matter type.

7.3.3 Dependence on Ambiguities

Any mechanism to avoid singularities must happen or at least mainly apply in strong quantum regimes. It may thus be sensitive to ambiguities such as factor ordering choices which have no classical analog. As an example, we look at the volume quantization in loop quantum cosmology, which has an influence not just on the dynamical approach to a singularity (the volume operator features prominently in the dynamics) but also on the identification of homogeneous singularities as states annihilated by the volume.

In analyzing inverse-triad corrections, here and in cosmological applications of the corrected perturbation equations of Chap. 10, we mostly use the behavior for larger values of μ where correction functions (3.59) drop off to the classical value one, as in Fig. 3.3. On very small scales, the approach to zero at $\mu = 0$ is characteristic for operators with U(1)-holonomies as they appear in homogeneous models or in the perturbative treatment. In particular, as we have seen explicitly in isotropic models the volume operator $\hat{V}$ and gauge-covariant combinations of commutators such as $\mathrm{tr}(\tau^i \hat{h}[\hat{h}^{-1}, \hat{V}])$ commute. It is thus meaningful to speak of the (eigen-)value of inverse volume on zero-volume eigenstates. For non-Abelian holonomies such as those for SU(2) in the full theory, the operators become non-commuting [40]. The inverse volume at zero-volume eigenstates thus becomes unsharp and one can at most make statements about expectation values rather than eigenvalues, which again requires more information on suitable states. Then, the expectation values are not expected to become sharply zero at zero volume, as calculations indeed show [41] (using a kinematical notion of coherent states). In addition, also here quantization ambiguities matter: We can write volume itself, and not just inverse volume, through Poisson brackets such as [40]

$$V = \int \mathrm{d}^3x \left(\frac{\varepsilon^{abc}\varepsilon_{ijk}}{6(10\pi\gamma G/3)^3} \int \mathrm{d}^3y_1 \{A_a^i(x), |\det e(y_1)|^{5/6}\} \right.$$
$$\left. \times \int \mathrm{d}^3y_2 \{A_b^j(x), |\det e(y_2)|^{5/6}\} \int \mathrm{d}^3y_3 \{A_c^j(x), |\det e(y_3)|^{5/6}\} \right)^2 .$$

After regularization, splitting the integration into sums over small patches of coordinate size ℓ_0^3 with volume contributions $V_v \approx \ell_0^3 |\det(e_a^i)|$, we obtain

$$V_v = \ell_0^6 \left(\frac{|\det e|}{\sqrt{V_v}} \right)^2 = \ell_0^6 \left(\varepsilon^{abc}\varepsilon_{ijk} \frac{e_a^i}{V_v^{1/6}} \frac{e_b^j}{V_v^{1/6}} \frac{e_c^k}{V_v^{1/6}} \right)^2$$
$$= \left(\frac{\varepsilon^{abc}\varepsilon_{ijk}}{6(10\pi\gamma G/3)^3} \ell_0^3 \{A_a^i, V_v^{5/6}\}\{A_b^j, V_v^{5/6}\}\{A_c^j, V_v^{5/6}\} \right)^2$$

whose quantization, making use of commutators, differs from the original volume operator of loop quantum gravity. If non-Abelian holonomies are used, the new volume operator does not commute with the full volume operator of [7] or [8]. This clearly shows that the usual quantization ambiguity in writing inverse-triad expressions also applies to what is considered the relevant geometrical volume. (Related ambiguities for flux operators have been discussed in [42].) For geometrical properties one may not only consider the original volume operator constructed directly from fluxes, but any operator having volume as the classical limit. In order to find zero-volume states to be related to classical singularities, the general fundamental dynamics of the form (4.15) indicates that operators constructed through commutators with the original volume operator are more relevant than the volume operator constructed directly from fluxes [40]. Thus, as one example of the relevance of quantization ambiguities for questions of singularity removal, specific volume eigenstates have to be used with great care in applications with non-Abelian holonomies.

7.4 Negative Attitude

Singularity removal in general terms may depend sensitively on specific properties of the quantum state of the universe which is not under observational control. This problem applies to the question whether singularities are removed, but also to how specifically resolution would be achieved. In such a situation, a "negative attitude" is useful, where one tries to quantify limitations to what can actually be said in detail, and to find out which possibilities remain within the bounds. An example is the analysis of asymmetries of states before and after a bounce of the solvable model, as already discussed in detail. Continuing such an analysis in this and other models will show clearly how much the small-volume behavior of quantum cosmology can be elucidated, and which questions must remain open. The derivations of strong symmetry bounds in highly specific or even solvable models, by contrast, is much less relevant because it does not show how the behavior may be restricted in realistic situations.

Several results in loop quantum cosmology can be seen to be investigated along the viewpoint of negative attitude. For instance, singularities in tree-level equations have been identified in scalar models, which are not big-bang but sudden future singularities [43]. While the analysis based on tree-level equations would still have to be justified by a detailed derivation of effective equations with the potential used, as a negative result the statement is of interest: it shows the limitations of tree-level equations and what quantum back-reaction terms would have to provide to achieve non-singular behavior in that case. Also, extending c^2 in the isotropic Hamiltonian constraint to almost-periodic functions in more complicated ways than normally done can lead to new types of singularities of diverging Hubble parameter even before the high-density regime of the holonomy-induced bounce is reached [44]. Such studies show how generic the singularity-resolution mechanisms of loop quantum cosmology are.

Similarly, possible cases of the large-volume behavior have been studied with a parameterized form for the growth of quantum fluctuations. The model used was actually the solvable one, where explicit solutions for the behavior of fluctuations are available, but with a different factor ordering. What was found by the parameterization was that the behavior of fluctuations can be very important for the large-volume behavior, too, even in the absence of a positive cosmological constant as we discussed it earlier. If the wrong behavior of fluctuations is used, even a flat model can lead to a recollapse at large volume in disagreement with the expected classical limit [45, 46]. This is true even for a behavior of fluctuations that would still allow one to interpret states as semiclassical. The analysis underlines the importance of considering the exact state properties for effective equations, rather than picking a certain form of dynamical fluctuations or correlations. All quantum variables must be evolved from their initial values onwards to ensure that the correct dynamics, also of expectation values, is captured.

The distinguishing feature of those examples is that they show possible limitations to proposed singularity-avoidance mechanisms, rather than providing more examples of the same special scenario such as a bounce. As the theory is further developed, instances of possible breaches, rather than superficial uniqueness claims of simple mechanisms, will be very valuable to probe its general behavior.

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